Numerical Optimisation
Nonsmooth optimisation

Marta M. Betcke
m.betcke@ucl.ac.uk,

Kiko Rullan
f.rullan@cs.ucl.ac.uk

Department of Computer Science,
Centre for Medical Image Computing,
Centre for Inverse Problems
University College London

Lecture 16

Subgradient

For convex differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ it holds

$$f(y) \geq f(x) + \nabla f(x)^{\mathrm{T}}(y - x).$$

A vector $g \in \mathbb{R}^n$ is a **subgradient** of a function f at $x \in \operatorname{dom} f$ if

$$f(y) \geq f(x) + g^{\mathrm{T}}(y - x) \quad \forall y \in \operatorname{dom} f.$$

- $f(x) + g^{\mathrm{T}}(y - x)$ is affine global underestimator
- g is a subgradient of f at x if $(g, -1)$ supports the epigraph of f at $(x, f(x))$

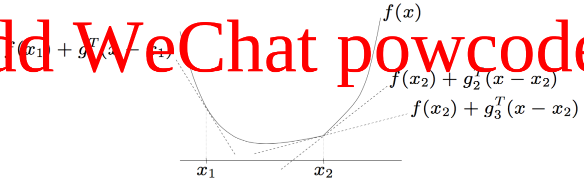


Figure: $\partial f(x_1) = \{\nabla f(x_1)\} = \{g_1\}$, $\partial f(x_2) = [g_3, g_2]$. Fig. from S. Boyd, EE364b, Stanford University.

Subdifferential

A function f is called **subdifferentiable** at x if there exists at least one subgradient at x.

Subdifferential of f at x, $\partial f(x)$, is the set of all subgradients of f at x.

$\partial f(x)$ is a closed convex set (can be empty) even if f is not convex.
Proof: It follows from it being intersection of infinite set of halfspaces

$$\partial f(x) = \bigcap_{z \in \operatorname{dom} f} \{g : \ f(z) \geq f(x) + g^{\mathrm{T}}(z - x)\}.$$

If $f(x)$ is convex

- $\partial f(x)$ is nonempty for $x \in \operatorname{relint} \operatorname{dom} f$
- then f is continuous at x, and hence the $\partial f(x)$ is bounded
- $\partial f(x) = \{\nabla f(x)\}$ iff f differentiable at x

A point $x^\star$ is a minimiser of a function f (not necessarily convex) iff f is subdifferentiable at $x^\star$ and

$$0 \in \partial f(x^\star),$$

i.e. $g = 0$ is a subgradient of f at $x^\star$.

Proof: This follows directly from $f(x) \geq f(x^\star)$ for all $x \in \operatorname{dom} f$.
f is subdifferentiable at $x^\star$ with $0 \in \partial f(x^\star)$ is equivalent to $f(x) \geq f(x^\star) + 0^{\mathrm{T}}(x - x^\star)$ for all $x \in \operatorname{dom} f$.

The condition $0 \in \partial f(x^\star)$ reduces to $\nabla f(x^\star) = 0$ when f is convex and differentiable at $x^\star$. Note, that in that case also it is a necessary and sufficient condition.

Convex constraint optimisation problem

$$\min_{x \in \mathbb{R}^n} \quad f(x) \tag{COP}$$

$$\text{subject to} \quad f_i(x) \leq 0, \quad i = 1, \dots, m,$$

where

- $f, f_i : \mathbb{R}^n \to \mathbb{R}$ is convex hence subdifferentiable
- strict feasibility holds (Slater's conditions)

Generalised KKT conditions:

$x^\star$ is primal optimal and $\lambda^\star$ dual optimal iff

$$
\begin{aligned}
f_i(x^\star) &\leq 0, \\
\lambda_i^\star &\geq 0, \\
0 &\in \partial f(x^\star) + \sum_{i=1}^{m} \lambda_i^\star \partial f_i(x^\star), \\
\lambda_i^\star f_i(x^\star) &= 0
\end{aligned} \tag{KKT}
$$

Directional derivatives and subdifferential

For a convex function the *directional derivative* at x in the direction v is

$$f'(x;v) = \lim_{t \to 0} \frac{f(x+tv) - f(x)}{t}.$$

The limit always exists for a convex function, thought it can be $\pm\infty$. If f is finite in a neighbourhood of x, then $f'(x;v)$ exists.

f is differentiable at x iff for some g (which is $\nabla f(x)$) and all $v \in \mathbb{R}^n$ we have $f'(x;v) = g^{\mathrm{T}} v$ ($f'(x;v)$ is a linear function of v).

The directional derivative $f'(x;v)$ of a convex function f satisfies

$$f'(x;v) = \sup_{g \in \partial f(x)} g^{\mathrm{T}} v.$$

Proof idea: Note that $f'(x;v) \geq \sup_{g \in \partial f(x)} g^{\mathrm{T}} v$ by the definition of the subgradient $f(x+tv) - f(x) \geq t g^{\mathrm{T}} v$ for any $t \in \mathbb{R}$ and $g \in \partial f(x)$. Other direction: show that all affine functions below $v \to f'(x;v)$ may be taken to be linear.

Weak subgradient calculus: formulas for finding *one* $g \in \partial f(x)$.
If you can compute f, you can usually compute one subgradient.
Many algorithms require only one subgradient.

Strong subgradient calculus: formular for finding *the whole* subdifferential $\partial f(x)$
Optimality conditions and some algorithms require the whole differential.

Basic rules:

- scaling: for $\alpha > 0$, $\partial(\alpha f) = \alpha \partial f$
- addition: $\partial(f_1 + f_2) = \partial(f_1) + \partial(f_2)$
- affine transformation: $g(x) = f(Ax + b)$, $\partial g(x) = A^{\mathrm{T}} \partial f(Ax + b)$
- finite point wise maximum: $f = \max_{i=1,\dots,m} f_i$, $\partial f(x) = \mathbf{Co} \bigcup \{\partial f_i(x) : \ f_i(x) = f(x)\}$ (convex hull of a union of subdiffrentials of active functions at x)

Subgradient and descent direction

p is a descent direction for f at x if $f'(x;p) < 0$.

If f is differentiable, $-\nabla f$ is always a descent direction (except when it is 0).

For a nondifferentiable convex function f, $p = -g$, $g \in \partial f(x)$ need not to be a descent direction.

Example: $f(x) = |x_1| + 2|x_2|$

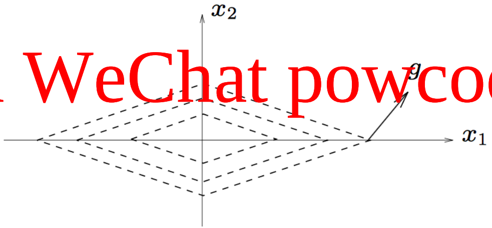


Figure: Fig. from S. Boyd, EE364b, Stanford University.

For a convex f, if $f(z) < f(x)$, $g \in \partial f(x)$, then for small $t > 0$

$$\|x - tg - z\|_2 < \|x - z\|_2.$$

Thus $-g$ is descent direction for $\|x - z\|_2$, for any z with $f(z) < f(x)$.

Proof:

$$\begin{aligned} \|x - tg - z\|_2^2 &= \|x - z\|_2^2 - 2tg^{\mathrm{T}}(x - z) + t^2\|g\|_2^2 \\ &\le \|x - z\|_2^2 - 2t\underbrace{(f(x) - f(z))}_{>0} + \underbrace{t^2\|g\|_2^2}_{t:\ \frac{t}{2}\|g\|_2^2 < f(x) - f(z)} \end{aligned}$$

In particular, choosing $z = x^\star$, we obtain that the negative subgradient is a descent direction for distance to optimal point $x^\star$.

Proximal operator

Proximal operator of $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$

$$\mathrm{prox}_{\lambda f}(v) := \arg\min_x \left(f(x) + 1/(2\lambda)\|x - v\|_2^2 \right), \ \lambda > 0 \quad \text{(PROX)}$$

Evaluating prox_f involves solving a convex optimisation problem.

Can evaluate numerically via e.g. BFGS, but often the convex problem (PROX) has an analytical solution or at least a specialised linear-time algorithm.

Indicator function of a closed convex set, $\mathcal{C} \neq \emptyset$

$$I_{\mathcal{C}}(x) = \begin{cases} 0 & x \in \mathcal{C} \\ \infty & \text{otherwise} \end{cases}$$

Proximal operator of $I_{\mathcal{C}}$ is the Euclidean projection

$$\mathrm{prox}_{\lambda I_{\mathcal{C}}}(v) = \arg\min_{x \in \mathcal{C}} \|x - v\|_2 = \Pi_{\mathcal{C}}(v)$$

Many properties of projection carry over to proximal operator.

Important special choices of f, for which $\mathrm{prox}_{\lambda f}$ has a closed form:

- $f(x) = \frac{1}{2}\|Px - q\|_2^2$,

$$\mathrm{prox}_{\lambda f}(v) = (P^{\mathrm{T}}P + \lambda^{-1}I)^{-1}(P^{\mathrm{T}}q + \lambda^{-1}v).$$

$$(P^{\mathrm{T}}P + Q)^{-1} = Q^{-1} - Q^{-1}P^{\mathrm{T}}(I + PQ^{-1}P^{\mathrm{T}})^{-1}PQ^{-1}.$$

- f is separable i.e. $f(x) = \sum_i^n f_i(x_i)$, proximal operator acts componentwise

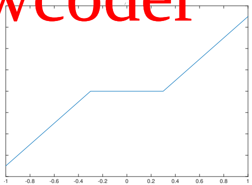
$$(\mathrm{prox}_{\lambda f}(v))_i = \mathrm{prox}_{\lambda f_i}(v_i), \quad i = 1, \dots, n$$

- $f(x) = \|x\|_1$

$$\mathrm{prox}_{\lambda f}(v) = S_\lambda(v),$$

with elementwise soft thresholding

$$S_\delta(x) = \begin{cases} x - \delta & x > \delta \\ 0 & x \in [-\delta, \delta] \\ x + \delta & x < -\delta \end{cases}$$



Another important example which does not admit close form is Total Variation, $f(x) = TV(x)$, defined as follows

$$
\begin{aligned}
TV(x) \quad := \quad & \sum_{i=1}^{m-1} \sum_{j=1}^{n-1} \sqrt{(x_{i,j} - x_{i+1,j})^2 + (x_{i,j} - x_{i,j+1})^2} \\
& + \sum_{i=1}^{m-1} |x_{i,n} - x_{i+1,n}| + \sum_{i=1}^{n-1} |x_{m,j} - x_{m,j+1}|
\end{aligned}
$$

assuming standard reflexive boundary conditions

$$
x_{m+1,j} = x_{m,j}, \quad x_{i,n+1} = x_{i,n}.
$$

The proximal operator has to be computed iteratively using e.g. Chambolle-Pock algorithm (primal dual proximal gradient).

Resolvent of subdifferential operator

Proximal operator

$$\mathrm{prox}_{\lambda f}(v) = \arg\min_x \left(f(x) + 1/(2\lambda)\|x - v\|_2^2\right).$$

The first order condition for the minimiser reads

$$\begin{aligned} 0 &\in \partial f(x) + 1/\lambda(x - v) \\ v &\in \lambda \partial f(x) + x \\ v - x &\in \lambda \partial f(x) \\ \mathrm{prox}_{\lambda f}(v) &= (I + \lambda \partial f)^{-1} v \end{aligned}$$

Mapping $(I + \lambda \partial f)^{-1}$ is called **resolvent** of operator ∂f.

$x^\star$ minimises f iff $x^\star$ is a fixed point

$$x^\star = \mathrm{prox}_f(x^\star)$$

Moreau envelope or **Moreau-Yosida regularisation** of f

$$M_{\lambda f}(v) = \inf_x \left(f(x) + 1/(2\lambda)\|x - v\|_2^2 \right).$$

$M_{\lambda f}$ is a smoothed (regularised) version of f:

- always has full domain
- always continuously differentiable
- has the same minimisers as f

Can show that $M_f = (f^\star + 1/2\|\cdot\|_2^2)^\star$.

Example: Moreau envelope of $|\cdot|$ is the Huber function

$$M_{|\cdot|}(x) = \begin{cases} x^2 & |x| \le 1 \\ 2|x| - 1 & |x| > 1 \end{cases}$$

Moreau decomposition: $v = \mathrm{prox}_f(v) + \mathrm{prox}_{f^\star}(v)$ is generalisation of orthogonal decomposition $v = \Pi_W(v) + \Pi_{W^\perp}(v)$.
It follows from Moreau decomposition that $(I_W)^\star = I_{W^\perp}$.

$$\min_x f(x) + g(x) \quad \text{subject to } x \in \mathbb{E} \tag{1}$$

- $\mathbb{E}$: finite dimensional Euclidean space with inner product $< \cdot, \cdot >$ and self dual norm $\| \cdot \| =< \cdot, \cdot >^{1/2} = \| \cdot \|_*$, e.g. space of $n \times m$ images, $\mathbb{R}^{n \times m}$
- $f : \mathbb{E} \to \mathbb{R}$ continuously differentiable with Lipschitz continuous gradient, $\|\nabla f(x) - \nabla f(y)\| \leq L(f)\|x - y\|, \ \forall x, y \in \mathbb{E}$.
- $g : \mathbb{E} \to (-\infty, \infty]$ proper closed convex.

From first order optimality condition we have

$$\begin{aligned}
0 &\in \nabla f(x^*) + \partial g(x^*) \\
0 &\in \tau \nabla f(x^*) + \tau \partial g(x^*) - x^* + x^* \\
(I + \tau \partial g)(x^*) &\in (I - \tau \nabla f)(x^*) \\
x^* &= (I + \tau \partial g)^{-1}(I - \tau \nabla f)(x^*) \qquad (2)
\end{aligned}$$

Iterative scheme:

$$\begin{aligned} x_k &= \operatorname{prox}_{\tau_k g}(x_{k-1} - \tau_k \nabla f(x_{k-1})) \\ &= \arg\min_x \left\{ g(x) + \frac{1}{2\tau_k} \|x - (x_{k-1} - \tau_k \nabla f(x_{k-1}))\|^2 \right\}. \end{aligned}$$

- **Gradient Projection:** $g(x) = I_{\mathcal{C}}(x)$: smooth constrained minimisation, $\tau_k \in (0, 2/L(f))$

$$x_k = \Pi_{\mathcal{C}}(x_{k-1} - \tau_k \nabla f(x_{k-1})).$$

- **Proximal Minimization:** $f(x) = 0$: non-smooth convex minimisation

$$x_k = \arg\min_x \left\{ g(x) + \frac{1}{2\tau_k} \|x - x_{k-1}\|^2 \right\}.$$

- **Iterative Shrinkage Thresholding Algorithm (ISTA):** $g(x) = \|x\|_1$, $f(x) = \|Ax - b\|^2$, $\tau_k \in (0, 2/L(f))$

$$x_k = S_{\tau_k}(x_{k-1} - \tau_k \nabla f(x_{k-1})).$$

$$
\begin{aligned}
x_k &= \mathrm{prox}_{\tau_k g}(x_{k-1} - \tau_k \nabla f(x_{k-1})) \\
&= \arg\min_x \left\{ g(x) + \frac{1}{2\tau_k} \| x - (x_{k-1} - \tau_k \nabla f(x_{k-1})) \|^2 \right\}.
\end{aligned}
$$

- **Gradient Projection:** $g(x) = I_{\mathcal{C}}(x)$: smooth constrained minimisation, $\tau_k \in (0, 2/L(f))$
$$x_k = \Pi_{\mathcal{C}}(x_{k-1} - \tau_k \nabla f(x_{k-1})).$$

- **Iterative Shrinkage Thresholding Algorithm (ISTA):** $g(x) = \|x\|_1$, $f(x) = \|Ax - b\|^2$, $\tau_k \in (0, 2/L(f))$
$$x_k = S_{\tau_k}(x_{k-1} - \tau_k \nabla f(x_{k-1})).$$

Slow convergence, if $\tau_k = \tau = 1/L$, $L \geq L(f)$

$$F(x_k) - F^* \leq \frac{L\|x_0 - x^*\|^2}{2k}.$$

Fast Iterative Shrinkage Thresholding Algorithm (FISTA):

Initialize: $y_1 := x_0 \in \mathbb{E}, \ \tau_1 = 1$.

$$\text{Step } k: \qquad x_k = \mathrm{prox}_{1/L}(g)\left(y_k - \frac{1}{L}\nabla f(y_k)\right)$$

$$\tau_{k+1} = \frac{1 + \sqrt{1 + 4\tau_k^2}}{2}$$

$$y_{k+1} = x_k + \frac{\tau_k - 1}{\tau_{k+1}}(x_k - x_{k-1}).$$

Convergence, if $\tau_k = \tau = 1/L$, $L \geq L(f)$

$$F(x_k) - F^* \leq \frac{2L\|x_0 - x^*\|^2}{(k+1)^2}.$$

Fast Projection Gradient [Nesterov'83]: $g(x) = I_{\mathcal{C}}(x)$

$$x_k = \Pi_{\mathcal{C}}\left(y_k - \frac{1}{L}\nabla f(y_k)\right).$$

More details on Nesterov algorithm see e.g. `http://www.seas.ucla.edu/~vandenbe/236C/lectures/fgrad.pdf`

Review: Optimisation with equality constraints

Let $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$, closed, proper and convex.

Primal problem

$$\min_x f(x) \quad \text{subject to } Ax = b$$

Lagrangian

$$\mathcal{L}(x, y) = f(x) + y^T(Ax - b)$$

Dual function

$$g(y) = \inf_x \mathcal{L}(x, y) = -f^*(-A^{\mathrm{T}}y) - b^{\mathrm{T}}y$$

y: dual variable (Lagrange multiplier),
f^*: convex conjugate of f (f^* is convex and closed even if f is not).

Dual problem (always concave, $y^* \leq x^*$, $y^* = x^*$ if strong duality holds)

$$\max_y g(y). \tag{3}$$

Gradient descent for primal problem (assuming f continuously differentiable)

$$x_{k+1} = x_k - \tau_k \nabla f(x_k)$$

Gradient ascent for dual problem (assuming g continuously differentiable)

$$\begin{aligned} x_{k+1} &= \arg\min_x L(x, y_k) \\ y_{k+1} &= y_k + \tau_k \underbrace{(Ax_{k+1} - b)}_{=\nabla g(y_k)} \end{aligned}$$

Remark: the primal update is part of evaluation of $\nabla g(y_k)$

+ for separable f it leads to a parallel algorithm.
– various conditions necessary for convergence e.g. strict convexity of f, $f(x) < \infty, \forall x$.

Augmented Lagrangian

$$\mathcal{L}_\rho(x,y) = f(x) + y^{\mathrm{T}}(Ax-b) + \rho/2\|Ax-b\|_2^2, \quad \rho > 0 \quad \text{(AL)}$$

Equivalent to Lagrangian of an equivalent problem (for all feasible x the quadratic term equals 0)

$$\min_x f(x) + \rho/2\|Ax-b\|_2^2, \quad \text{subject to } Ax = b.$$

Method of multipliers (MM): dual ascent applied to (AL)

$$\begin{aligned} x_{k+1} &= \arg\min \mathcal{L}_\rho(x, y_k) \\ y_{k+1} &= y_k + \rho \underbrace{(Ax_{k+1} - b)}_{=\nabla g(y_k)} \end{aligned}$$

Using ρ at a step size guarantees dual feasibility of (x_{k+1}, y_{k+1}):
$0 = \nabla_x \mathcal{L}_\rho(x_{k+1}, y_k) = \nabla f(x) + A^{\mathrm{T}} y_k + \rho A^{\mathrm{T}}(Ax-b)\big|_{x=x_{k+1}} =$
$\nabla f(x_{k+1}) + A^{\mathrm{T}} y_{k+1} =: s_{k+1} = 0.$

+ converges under more general conditions

– augmented Lagrangian is non-separable.

Blend separability of dual ascent with superior convergence of MM:

$$\min_{x\in\mathbb{R}^n,\, z\in\mathbb{R}^m} f(x) + g(z) \quad \text{subject to } Ax + Bz = c \tag{4}$$

with $A \in \mathbb{R}^{p\times n}$, $B \in \mathbb{R}^{p\times m}$, $c \in \mathbb{R}^p$ and $g : \mathbb{R}^m \to \mathbb{R} \cup \{+\infty\}$ closed, proper and convex.

The equality constraint comes from the split of the variable into x and z with the objective function separable across the splitting.

Augmented Lagrangian

$$L_\rho(x, z, y) = f(x) + g(z) + y^{\mathrm{T}}(Ax + Bz - c) + \rho/2\|Ax + Bz - c\|_2^2,$$

ADMM

$$\begin{aligned} x_{k+1} &= \arg\min_x L_\rho(x, z_k, y_k) \\ z_{k+1} &= \arg\min_z L_\rho(x_{k+1}, z, y_k) \\ y_{k+1} &= y_k + \rho(Ax_{k+1} + Bz_{k+1} - c). \end{aligned}$$

Blend separability of dual ascent with superior convergence of MM:

$$\min_{x\in\mathbb{R}^n,\, z\in\mathbb{R}^m} f(x)+g(z) \quad \text{subject to } Ax+Bz=c \tag{4}$$

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Augmented Lagrangian

$$L_\rho(x,z,y) = f(x)+g(z)+y^{\mathrm{T}}(Ax+Bz-c)+\rho/2\|Ax+Bz-c\|_2^2,$$

Dual ascent on $\mathcal{L}_\rho$ (joint minimisation)

$$(x_{k+1}, z_{k+1}) = \arg\min_{x,z} L_\rho(x,z,y_k)$$

$$y_{k+1} = y_k + \rho(Ax_{k+1}+Bz_{k+1}-c).$$

Augmented Lagrangian

$$
\begin{aligned}
L_\rho(x,z,y) &= f(x) + g(z) + y^{\mathrm{T}}\underbrace{(Ax+Bz-c)}_{=:r} + \rho/2\|\underbrace{Ax+Bz-c}\|_2^2, \\
&= f(x) + g(z) + y^{\mathrm{T}} r + \rho/2\|r\|_2^2. \\
&= f(x) + g(z) + \rho/2\|r+u\|_2^2 - \rho/2\|\underbrace{u}_{:=(1/\rho)y}\|_2^2,
\end{aligned}
$$

with $u = (1/\rho)y$ the *scaled dual variable*.

ADMM: scaled form

$$
\begin{aligned}
x_{k+1} &= \arg\min_x f(x) + \rho/2\|Ax + Bz_k - c + u_k\|_2^2 \\
z_{k+1} &= \arg\min_z g(z) + \rho/2\|Ax_{k+1} + Bz - c + u_k\|_2^2 \\
u_{k+1} &= u_k + Ax_{k+1} + Bz_{k+1} - c.
\end{aligned}
$$

Assume in addition that the unaugmented Lagrangian $\mathcal{L}$ has a saddle point.

For f, g proper, closed, convex, it follows that strong duality holds (no explicit assumptions on A, B, c).

Under these assumptions the ADMM iterates satisfy

- Residual convergence: $r^k \to 0$ as $k \to \infty$ i.e. the iterates approach feasibility.
- Objective convergence: $f(x^k) + g(z^k) \to p^\star$ as $k \to \infty$ i.e. the objective function of the iterates approach the optimal value

- Dual variable convergence: $y^k \to y^\star$ as $k \to \infty$, where $y^\star$ is a dual optimal point.

Note, that x^k, z^k need not converge to optimal points, although such a result can be shown under additional assumptions.

Optimality conditions

Necessary and sufficient optimality conditions for ADMM

$$
\begin{aligned}
Ax^\star + Bz^\star - c &= 0 \quad \text{primal feasibility} \\
0 &\in \partial f(x^\star) + A^{\mathrm{T}} y^\star \quad \text{dual feasibility} \\
0 &\in \partial g(z^\star) + B^{\mathrm{T}} y^\star \quad \text{dual feasibility}
\end{aligned}
$$

As for MM, it follows from $z_{k+1} = \arg\min_z \mathcal{L}_\rho(x_{k+1}, z, y_k)$ that z_{k+1} and y_{k+1} always satisfy the last equation.

From $x_{k+1} = \arg\min_x \mathcal{L}_\rho(x, z_k, y_k)$ we have

$$
\begin{aligned}
0 &\in \partial f(x_{k+1}) + A^{\mathrm{T}} y_k + \rho A^{\mathrm{T}}(Ax_{k+1} + Bz_{k+1} - c) \\
&= \partial f(x_{k+1}) + A^{\mathrm{T}}(y_k + \rho r_{k+1} + \rho B(z_k - z_{k+1})) \\
&= \partial f(x_{k+1}) + A^{\mathrm{T}} y_{k+1} + \rho A^{\mathrm{T}} B(z_k - z_{k+1})
\end{aligned}
$$

or equivalently

$$s_{k+1} := \rho A^{\mathrm{T}} B(z_{k+1} - z_k) \in \partial f(x_{k+1}) + A^{\mathrm{T}} y_{k+1},$$

which can be interpreted as dual feasibility condition and s_{k+1} is the *dual residual* at iteration $k+1$.

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